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Structure investigation of mesalazine drug using thermal analyses, mass spectrometry, DFT calculations, and NBO analysis

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Abstract Mesalazine (MZ) drug has been used for several decades as a primary treatment for inflammatory bowel diseases. The drug was investigated using thermal analysis (TA) measurements and electron impact mass spectral fragmentation at 70 and 15 eV of electron energy. The optimum molecular geometry and the total energy of the neutral and the positively charged MZ molecules were calculated by density functional theory method with 6-311++G(d,p) basis sets. Stability of the molecules arising from hyperconjugative interactions, charge delocalization, and the natural atomic charges has been analyzed using natural bond orbital analysis. In electron ionization mass spectrometry, the primary rupture is due to successive loss of H_2O (OH from carboxyl and H from phenolic OH of the ring) and CO of the acetyl group. Thermogravimetric results have revealed two stages of mass loss at 75.3 and 25.3 % in ranges 225–350 and

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